

# Spinodal Decomposition and the Tomita Sum Rule

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The scaling properties of a phase-ordering system with a conserved order parameter are studied. The theory developed leads to scaling functions satisfying certain general properties including the Tomita sum rule. The theory also gives good agreement with numerical results for the order parameter scaling function in three dimensions. The values of the associated nonequilibrium decay exponents are given by the known lower bounds.

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## I. INTRODUCTION

In the area of phase-ordering kinetics [1] there are a wide variety of systems which satisfy a form of dynamical scaling. In the case of systems with a nonconserved order parameter (NCOP) we have a simple approximate theoretical model due to Ohta, Jasnow and Kawasaki [2] (OJK) which captures the main scaling properties of the associated physical systems. In the case of a conserved order parameter (COP) the situation is much less satisfactory. The difficulty in the COP case is that there are competing length scales which lead to the necessity of treating crossover. This crossover connects up the short-scaled-distance nonanalytic domain wall behavior associated with Porod's law [3–5] and the large distance constraints of the conservation law. A theory is offered in this paper which is consistent with all of the prominent scaling features in the case of a conserved scalar order parameter.

An auxiliary field method is used in essentially all the available explicit calculations of scaling functions in phase-ordering kinetics. Thus in the OJK approach [2,6–9], and our previous work [10–12], a local mapping from the original order parameter  $\psi$  onto an approximately gaussian variable  $m$  was developed. While these methods can be shown to work well for the NCOP case, there are

severe limitations in the COP case. In particular Yeung, Oono and Shinozaki [13] found that such a local mapping in the COP case led to mathematically unacceptable results within the theory. All of these theories were developed with the idea that the mapping,  $\psi \rightarrow \psi(m)$ , leads to an equation of motion for  $m$  which could be argued to be approximately consistent with a gaussian distribution for  $m$ . In Refs. ([14]) and ([15]) a different approach was taken in treating the NCOP case. It was shown that the equation of motion for the auxiliary field  $m$  can be constructed with appeal only to the form of the growth law, defined below, and certain general symmetry constraints. Using a novel expansion method it was shown how one could obtain the OJK result in zeroth order of a systematic expansion. Higher order corrections for the associated nonequilibrium exponents were also obtained.

In this paper this general idea is applied to the simplest COP system given by the Cahn-Hilliard [16] (CH) model. One is led to introduce a nonlocal mapping between the order parameter and the auxiliary field and only certain general constraints on the theory, like the conservation law and the generalized form of the Tomita sum rule [17], are used to determine the parameters characterizing the nonlocal mapping and the correlation function for the underlying auxiliary field. Thus one has a nonlinear selection problem where one simultaneously constructs the parameters of the mapping and the scaling function. The selected scaling function is found to be in good agreement with the best available numerical results in three dimensions. The nonequilibrium exponents are also determined in this theory and take on values, as for the OJK theory, corresponding to the known [18] lower bounds.

## II. PHENOMENOLOGY

The equation of motion in the Cahn-Hilliard model governing the conserved scalar order param-

eter,  $\psi$ , is given in dimensionless form by:

$$\dot{\psi} = \nabla^2 (V'(\psi) - \nabla^2 \psi) \quad . \quad (1)$$

$V(\psi)$  is a degenerate double-well potential. Typically this system is driven by a set of uncorrelated random initial conditions. We look here at critical quenches where  $\langle \psi \rangle = 0$ . In this case the system is unstable and responds by locally growing competing degenerate patches of the stable low-temperature-ordered phases. These patches correspond to domains separated by sharp walls of width  $\xi$ . As time evolves these domains coarsen and the order grows to progressively longer length scales. The growth law,  $L(t)$ , increases without bound with time  $t$  after the quench. At long enough times  $L(t)$  dominates,  $L(t) \gg \xi$ , and the order parameter correlation function satisfies the scaling equation [19–21]

$$C(\mathbf{r}, t) \equiv \langle \psi(\mathbf{r}, t) \psi(0, t) \rangle = \psi_0^2 F(x) \quad (2)$$

where  $x \equiv r/L(t)$ , and  $\psi_0$  is the magnitude of  $\psi$  in the ordered state. The structure factor, the Fourier transform of  $C(\mathbf{r}, t)$ , satisfies

$$C(\mathbf{q}, t) = L^d \psi_0^2 F(Q) \quad , \quad (3)$$

where  $Q \equiv qL$  is a scaled wavenumber and  $d$  the number of spatial dimensions. There are a number of general properties a correct theory of the phase ordering CH model must satisfy [22,12]:

1. The growth law is given by the Lifshitz-Slyozov-Wagner [23] form:  $L \approx t^{1/3}$ . This result can be obtained a number of different ways [24–26] that are all consistent.

2. The scaled-structure factor  $F(Q)$  has a  $Q^4$  behavior [27] for small scaled wavenumbers  $Q$  directly reflecting the conservation law.

3. The scaled-structure factor satisfies Porod's law [3–6,28] for large scaled wavenumbers,  $F(Q) \approx Q^{-(d+1)}$ .

4. The scaled-structure factor also satisfies the Tomita [17,6] sum rules. The scaling function  $F(x)$  has no even terms, except the first, in its expansion in powers of  $x$ :

$$F(x) = 1 + F_1 x + F_3 x^3 + \dots \quad . \quad (4)$$

While there are theories which satisfy some of these requirements, there has been none so far which satisfies all four. Our goal here is to find the simplest theory for the COP case which does satisfy all of these properties and leads to an explicit form for

the scaled structure factor which can be compared to the best numerical determinations of  $F(Q)$ . The challenge is to match the small  $Q^4$  behavior for  $F(Q)$  with the large  $Q^{-4}$  behavior (in three dimensions) while preserving the Tomita sum rule. Our approach will be similar to that developed in Refs.( [14]) and ( [15]) but with some significant differences.

### III. AUXILIARY FIELD MAPPING FOR COP

As in previous work, we assume in the scaling regime that the order parameter can be decomposed into an ordering component, which contributes to the order parameter structure factor at  $\mathcal{O}(1)$ , and a fluctuating piece which is of higher order in powers of  $1/L(t)$ :

$$\psi = \tilde{\psi} + \Theta/L \quad (5)$$

where  $\Theta$  is  $\mathcal{O}(1)$ . Here we assume that the ordering component,  $\tilde{\psi}$ , can be written in the form:

$$\tilde{\psi} = \sigma(m + u) \quad , \quad (6)$$

where, as usual,  $\sigma(m)$  is the solution of the classical interfacial equation

$$\frac{d^2 \sigma}{dm^2} = V'(\sigma) \quad , \quad (7)$$

with the boundary conditions  $\lim_{m \rightarrow \pm\infty} \sigma(m) = \pm \psi_0$ . It turns out in this case that it is necessary to introduce two independent fields  $m$  and  $u$ . We will organize the theory such that  $m$  is treated as the auxiliary field which, as in the NCOP case, governs the short scaled distance physics associated with Porod's law and the Tomita sum rule. We will assume, as a first approximation, that  $m$  is a gaussian variable driven by an equation of motion of a general form compatible with scaling and with coefficients determined by selection processes described in detail below. The quantity  $\Theta$  is, in principle, to be determined as a function of the more fundamental variables  $m$  and  $u$ . In practice we will not need to construct the correlations for the field  $u$  explicitly or assume that it is a gaussian field.

If we insert the ansatz given by Eq.(5) into the equation of motion, Eq.(1), we obtain

$$\frac{\partial \tilde{\psi}}{\partial t} + \frac{\partial}{\partial t} \left( \frac{\Theta}{L} \right) = \nabla^2 \left( V'(\tilde{\psi} + \Theta/L) - \nabla^2 (\tilde{\psi} + \Theta/L) \right) \quad . \quad (8)$$

We can use scaling arguments to estimate the contributions of various terms. We explicitly assume that  $L(t) = L_0 t^{1/3}$  in the scaling regime. The first term on the left-hand side of Eq.(8),  $\frac{\partial \tilde{\psi}}{\partial t}$ , is of  $\mathcal{O}(L^{-3})$  in the scaling regime. Then we can estimate

$$\frac{\partial}{\partial t} \left( \frac{\Theta}{L} \right) \approx \mathcal{O}(L^{-4}) \quad (9)$$

and this term can be dropped when compared to the leading order in the equation of motion. Next we can expand

$$V'(\tilde{\psi} + \Theta/L) = V'(\tilde{\psi}) + V''(\tilde{\psi}) \frac{\Theta}{L} + \mathcal{O}(L^{-2}) \quad . \quad (10)$$

In comparing these two terms we have, using Eq.(6) and  $m \approx L$ , that

$$V'(\tilde{\psi}) = \frac{d^2 \sigma(m+u)}{dm^2} \approx \mathcal{O}(L^{-2}) \quad (11)$$

and the term proportional to  $V''(\tilde{\psi}) = V''(\psi_0) + \mathcal{O}(L^{-1})$  dominates at leading order for long times. Finally we have that the last term on the right hand side of Eq.(1),

$$\nabla^4 (\tilde{\psi} + \Theta/L) \approx \mathcal{O}(L^{-4}) \quad , \quad (12)$$

and can be dropped in Eq.(8). The equation of motion then reduces to the key result

$$\frac{\partial \tilde{\psi}}{\partial t} = \frac{\kappa_0}{L} \nabla^2 \Theta \quad . \quad (13)$$

where  $\kappa_0 \equiv V''(\psi_0) > 0$ .

The quantity  $\Theta$  is arbitrary except for the very important constraints that it be of  $\mathcal{O}(1)$  in the scaling regime and it must be consistent with the system ordering. It is at this stage that we realize that there is an apparent flexibility in the construction of the scaling solution. Since there is a belief that the scaling functions are universal, there must be mechanisms, like the nonlinear eigenvalue problem encountered in Ref. [10], which selects the scaling structures which do not directly depend on the physics at the smaller length scales. The key assumption in going forward is that the auxiliary field method can be used to describe the *inner* scaling regime and there is a crossover to an *outer* scaling regime dominated by the conservation law. The building blocks we can use to construct  $\Theta$ , which are compatible with this crossover and are of  $\mathcal{O}(1)$ , are  $\tilde{\psi}$  and  $\sigma(m)$ .

The simplest assumption [29] for the Fourier transform  $\Theta_q(t)$ , robust enough to give a satisfactory solution to the problem, is of the form:

$$\Theta_q(t) = \tilde{M}_q(t) \tilde{\psi}_q(t) - \tilde{N}_q(t) \sigma_q(t) \quad (14)$$

where  $\tilde{M}_q(t)$  and  $\tilde{N}_q(t)$  are functions to be determined. The equation of motion, Eq.(13), is given then by:

$$\frac{\partial \tilde{\psi}_q(t)}{\partial t} = -M_q(t) \tilde{\psi}_q(t) + N_q(t) \sigma_q(t) \quad (15)$$

where

$$M_q(t) = \frac{\kappa_0 q^2}{L(t)} \tilde{M}_q(t) \quad (16)$$

$$N_q(t) = \frac{\kappa_0 q^2}{L(t)} \tilde{N}_q(t) \quad . \quad (17)$$

We can easily obtain a partial solution to Eq.(15). Let us define the auxiliary quantity

$$U_q(t_1, t_2) = e^{\left( - \int_{t_2}^{t_1} d\tau M_q(\tau) \right)} \quad (18)$$

and write

$$\tilde{\psi}_q(t) = U_q(t, t_0) \chi_q(t) \quad . \quad (19)$$

Taking the time derivative of this expression we find

$$\frac{\partial \tilde{\psi}_q(t)}{\partial t} = -M_q(t) \tilde{\psi}_q(t) + U_q(t, t_0) \frac{\partial \chi_q(t)}{\partial t} \quad . \quad (20)$$

Comparing Eqs.(15) and (20), we obtain the equation for  $\chi_q(t)$ ,

$$U_q(t, t_0) \frac{\partial \chi_q(t)}{\partial t} = N_q(t) \sigma_q(t) \quad , \quad (21)$$

which can be rewritten as

$$\frac{\partial \chi_q(t)}{\partial t} = U_q(t_0, t) N_q(t) \sigma_q(t) \quad . \quad (22)$$

This equation has the solution

$$\chi_q(t) = \tilde{\psi}_q(t_0) + \int_{t_0}^t d\bar{t} U_q(t_0, \bar{t}) N_q(\bar{t}) \sigma_q(\bar{t}) \quad (23)$$

or

$$\tilde{\psi}_q(t) = U_q(t, t_0) \tilde{\psi}_q(t_0) + \int_{t_0}^t d\bar{t} U_q(t, \bar{t}) N_q(\bar{t}) \sigma_q(\bar{t}) \quad . \quad (24)$$

This nonlocal relationship between  $\tilde{\psi}_q(t)$  and  $\sigma_q(t)$  should be contrasted with the local mapping used in previous theories. Because of the nonlocality the criticism of local mappings in the COP case due to Yeung, Oono, and Shinozaki [13,30] is irrelevant for the discussion here.

Notice that we need to determine the functions  $M_q(t)$ ,  $N_q(t)$ , and the variance of the field  $m$ . Averages over  $m$  are discussed in more detail below. Focusing on  $N$  and  $M$ , for our purposes here, we only need these quantities in the scaling regime. Inspection of Eq.(18) shows that a general form compatible with scaling is given by

$$M_q(t) = \frac{\partial G(Q^2)}{\partial t} \quad (25)$$

where  $Q = qL(t)$ . Similarly,

$$N_q(t) = \frac{\partial G_0(Q^2)}{\partial t} \quad . \quad (26)$$

We can then write

$$\begin{aligned} M_q(t) &= \frac{\partial G(Q^2)}{\partial Q^2} \frac{\partial Q^2}{\partial t} = \frac{\partial G(Q^2)}{\partial Q^2} \frac{\partial}{\partial t} q^2 L_0^2 t^{2/3} \\ &= \frac{\partial G(Q^2)}{\partial Q^2} \frac{2}{3} \frac{Q^2}{t} \equiv \frac{2}{3} \frac{H(Q^2)}{t} \end{aligned} \quad (27)$$

where

$$H(Q^2) = Q^2 \frac{\partial G(Q^2)}{\partial Q^2} \quad . \quad (28)$$

Similarly,

$$N_q(t) = \frac{2}{3} \frac{H_0(Q^2)}{t} \quad . \quad (29)$$

For our purposes it will be sufficient to assume that  $H$  and  $H_0$  have power series forms:

$$H(Q) = \sum_{n=2} \gamma_n Q^n \quad (30)$$

$$H_0(Q) = \sum_{n=2} \gamma_n^0 Q^n \quad . \quad (31)$$

For reasons discussed below, we will work explicitly with a model where only  $\gamma_2$ ,  $\gamma_{10}$ ,  $\gamma_2^0$ , and  $\gamma_{10}^0$  are nonzero.

#### IV. STRUCTURE FACTOR

The quantity of central interest is the order parameter structure factor:

$$\begin{aligned} C(q, t_1, t_2) &= \langle \psi_q(t_1) \psi_{-q}(t_2) \rangle \\ &= \langle \tilde{\psi}_q(t_1) \tilde{\psi}_{-q}(t_2) \rangle \quad , \end{aligned} \quad (32)$$

where in the second line we recognize that in the scaling regime only the ordering component of the order parameter contributes to the structure factor. Inserting Eq.(24) for  $\tilde{\psi}_q(t_1)$  we obtain:

$$\begin{aligned} C(q, t_1, t_2) &= \langle \int_{t_0}^{t_1} d\bar{t}_1 U_q(t_1, \bar{t}_1) N_q(\bar{t}_1) \sigma_q(\bar{t}_1) \\ &\quad \times \int_{t_0}^{t_2} d\bar{t}_2 U_q(t_2, \bar{t}_2) N_q(\bar{t}_2) \sigma_q(\bar{t}_2) \rangle \\ &= \int_{t_0}^{t_1} d\bar{t}_1 U_q(t_1, \bar{t}_1) N_q(\bar{t}_1) \\ &\quad \times \int_{t_0}^{t_2} d\bar{t}_2 U_q(t_2, \bar{t}_2) N_q(\bar{t}_2) C_\sigma(q, \bar{t}_1, \bar{t}_2) \end{aligned} \quad (33)$$

where

$$C_\sigma(q, t_1, t_2) = \langle \sigma_q(t_1) \sigma_q(t_2) \rangle \quad . \quad (34)$$

Notice that we have assumed that the correlations with the initial state have decayed to zero for long times compared to the  $\mathcal{O}(1)$  terms contributing to the scaling function. We also note that  $C(q, t_1, t_2)$  depends only on the magnitude of  $\mathbf{q}$ .

The next step is to realize that  $C_\sigma(q, t_1, t_2)$ , which we calculate explicitly below, satisfies a scaling relation:

$$C_\sigma(q, t_1, t_2) = L^d(t_1, t_2) \psi_0^2 F_\sigma(qL(t_1, t_2), t_1, t_2) \quad . \quad (35)$$

Inserting Eq.(35) into Eq.(33) gives

$$\begin{aligned} C(q, t_1, t_2) &= \int_{t_0}^{t_1} d\bar{t}_1 U_q(t_1, \bar{t}_1) N_q(\bar{t}_1) \\ &\quad \times \int_{t_0}^{t_2} d\bar{t}_2 U_q(t_2, \bar{t}_2) N_q(\bar{t}_2) L^d(\bar{t}_1, \bar{t}_2) \psi_0^2 F_\sigma(qL(\bar{t}_1, \bar{t}_2), \bar{t}_1, \bar{t}_2) \end{aligned} \quad (36)$$

Let us now define

$$L_T^2(t_1, t_2) = \frac{1}{2} (L^2(t_1) + L^2(t_2)) \quad , \quad (37)$$

and choose a time  $T$  such that

$$L_T(t_1, t_2) = L(T) \quad . \quad (38)$$

Remembering  $L(t) = L_0 t^{1/3}$ , we have

$$T = \left( \frac{1}{2} (t_1^{2/3} + t_2^{2/3}) \right)^{3/2} \quad . \quad (39)$$

Clearly for  $t_1 = t_2 = t$ ,  $T = t$ . Now make the change of variables  $\bar{t}_1 = Ts_1$  and  $\bar{t}_2 = Ts_2$  in Eq.(36). This requires treatment of the quantity

$$L_T(\bar{t}_1, \bar{t}_2) = L_T(Ts_1, Ts_2)$$

$$= L(T)\ell(s_1, s_2) = L_T(t_1, t_2)\ell(s_1, s_2) \quad , \quad (40)$$

where

$$\ell(s_1, s_2) = \sqrt{\frac{1}{2}(s_1^{3/2} + s_2^{3/2})} \quad . \quad (41)$$

Eq.(36) then takes the form:

$$\begin{aligned} C(q, t_1, t_2) &= \psi_0^2 \int_{t_0/T}^{t_1/T} Tds_1 U_q(t_1, Ts_1) N_q(Ts_1) \\ &\quad \times \int_{t_0/T}^{t_2/T} Tds_2 U_q(t_2, \bar{t}_2) N_q(Ts_2) \\ &\quad \times L^d(Ts_1, Ts_2) F_\sigma(qL_T(t_1, t_2)\ell(s_1, s_2), Ts_1, Ts_2) \\ &= \psi_0^2 \int_{t_0/T}^{t_1/T} ds_1 U_q(t_1, Ts_1) \int_{t_0/T}^{t_2/T} ds_2 U_q(t_2, Ts_2) \\ &\quad \times TN_q(Ts_1) TN_q(Ts_2) L^d(T)\ell^d(s_1, s_2) \\ &\quad \times F_\sigma(Q\ell(s_1, s_2), Ts_1, Ts_2) \\ &= L^d(T)\psi_0^2 F(Q, t_1, t_2) \end{aligned} \quad (42)$$

where  $Q = qL_T(t_1, t_2) = qL(T)$  and the physical scaling function is given by

$$F(Q, t_1, t_2) = \int_{t_0/T}^{t_1/T} ds_1 U_q(t_1, Ts_1) \int_{t_0/T}^{t_2/T} ds_2$$

$$\times U_q(t_2, Ts_2) TN_q(Ts_1) TN_q(Ts_2)$$

$$\times \ell^d(s_1, s_2) F_\sigma(Q\ell(s_1, s_2), Ts_1, Ts_2) \quad . \quad (43)$$

We can simplify things a bit in the quantities  $U_q$ , defined by Eq.(18), where we have in the argument of the exponentials

$$\int_{Ts_1}^t d\tau M_q(\tau) = \int_{s_1}^{t/T} dz_1 M_q(Tz_1) \quad . \quad (44)$$

Inserting our general form for  $M_q$ , given by Eq.(27), we have

$$\begin{aligned} \int_{s_1}^{t/T} d\tau M_q(\tau) &= \int_{s_1}^{t/T} dz_1 \frac{2}{3} \frac{H(qL(Tz_1))}{Tz_1} \\ &= \frac{2}{3} \int_{s_1}^{t/T} \frac{dz_1}{z_1} H(Q\ell(z_1)) \end{aligned} \quad (45)$$

where  $\ell(z_1) = z_1^{1/3}$ , and similarly

$$TN_q(Ts_1) = T \frac{2}{3} \frac{H_0(Q\ell(s_1))}{Ts_1} = \frac{2}{3} \frac{H_0(Q\ell(s_1))}{s_1} \quad . \quad (46)$$

Then

$$U_q(t_1, Ts_1) = e^{\left(-\frac{2}{3} \int_{s_1}^{t_1/T} \frac{dz_1}{z_1} H(Q\ell(z_1))\right)} \quad , \quad (47)$$

and the scaling function is given by

$$\begin{aligned} F(Q, t_1, t_2) &= \int_{t_0/T}^{t_1/T} ds_1 U_q(t_1, Ts_1) \int_{t_0/T}^{t_2/T} ds_2 U_q(t_2, Ts_2) \\ &\quad \times \frac{2}{3} \frac{H_0(Q\ell(s_1))}{s_1} \frac{2}{3} \frac{H_0(Q\ell(s_2))}{s_2} \\ &\quad \times \ell^d(s_1, s_2) F_\sigma(Q\ell(s_1, s_2), Ts_1, Ts_2) \quad . \quad (48) \end{aligned}$$

We can then make one final change of integration variables to  $y_i = s_i^{2/3}$  ( $i = 1, 2$ ).. We have then

$$\ell(s_1, s_2) = \left( \frac{s_1^{2/3} + s_2^{2/3}}{2} \right)^{1/2}$$

$$= \left( \frac{y_1 + y_2}{2} \right)^{1/2} = \tilde{\ell}(y_1, y_2) \quad , \quad (49)$$

the equation for the scaling function becomes,

$$\begin{aligned}
F(Q, t_1, t_2) &= \int_{(t_0/T)^{2/3}}^{(t_1/T)^{2/3}} \frac{dy_1}{y_1} U_q(t_1, T y_1^{3/2}) \\
&\times \int_{(t_0/T)^{2/3}}^{(t_2/T)^{2/3}} \frac{dy_2}{y_2} U_q(t_2, T y_2^{3/2}) \\
&\times H_0(Q\sqrt{y_1}) H_0(Q\sqrt{y_2}) \\
&\times \tilde{\ell}^d(y_1, y_2) F_\sigma(Q\tilde{\ell}(y_1, y_2), T y_1^{3/2}, T y_2^{3/2}), \quad (50)
\end{aligned}$$

and, with  $\bar{y}_1 = z_1^{2/3}$  in the integral,

$$U_q(t_1, T y_1^{3/2}) = e^{\left(-\int_{y_1}^{(t_1/T)^{2/3}} \frac{dy_1}{y_1} H(Q\sqrt{y_1})\right)} . \quad (51)$$

For our simple polynomial model given by Eq.(30) we can carry out the  $\bar{y}_1$  integration in  $U_q$  explicitly.

## V. AUXILIARY FIELD SCALING FUNCTION

We must now work out the scaling properties of the field  $\sigma(m(\mathbf{r}, t))$  in the case where  $m$  is a gaussian variable. It is well known that in the scaling regime

$$\begin{aligned}
C_\sigma(\mathbf{r}_1, t_1, \mathbf{r}_2, t_2) &= \langle \sigma(m(\mathbf{r}_1, t_1)) \sigma(m(\mathbf{r}_2, t_2)) \rangle \\
&= \psi_0^2 \frac{2}{\pi} \sin^{-1} f_0(\mathbf{r}_1, t_1, \mathbf{r}_2, t_2) , \quad (52)
\end{aligned}$$

where

$$f_0(\mathbf{r}_1, t_1, \mathbf{r}_2, t_2) = \frac{C_0(\mathbf{r}_1, t_1, \mathbf{r}_2, t_2)}{\sqrt{S_0(t_1)S_0(t_2)}} , \quad (53)$$

$$C_0(\mathbf{r}_1, t_1, \mathbf{r}_2, t_2) = \langle m(\mathbf{r}_1, t_1) m(\mathbf{r}_2, t_2) \rangle , \quad (54)$$

and

$$S_0(t_1) = C_0(\mathbf{r}_1, t_1, \mathbf{r}_1, t_1) . \quad (55)$$

Thus we need to focus on the determination of the auxiliary field correlation function  $C_0$ .

Let us assume that the general equation of motion satisfied at gaussian level by the auxiliary field  $m$  has the local form in Fourier space:

$$\frac{\partial m_q(t)}{\partial t} = -\omega_q(t) m_q(t) \quad (56)$$

for  $t > t_0$ . Since the growth law is of the form  $L = L_0 t^{1/3}$ , we see that for a scaling result we must choose  $\omega_q(t) \approx \mathcal{O}(L^{-3})$ . Since we can estimate  $q \approx \mathcal{O}(L^{-1})$  in the scaling regime, we write quite generally that

$$\begin{aligned}
\omega_q(t) &= \alpha_0 \frac{1}{L^3} + \alpha_1 \frac{q}{L^2} + \alpha_2 \frac{q^2}{L} + \alpha_3 q^3 \\
&= \frac{1}{L^3} (\alpha_0 + \alpha_1 Q + \alpha_2 Q^2 + \alpha_3 Q^3) \quad (57)
\end{aligned}$$

where  $Q = qL$ . We can use general arguments, similar to those due to Ohta and Nozaki [31], to justify including the odd terms in  $Q$ . Eq.(57) can be rewritten in the convenient form

$$\omega_q(t) = \frac{\partial \Omega(Q(t))}{\partial t} - \omega_0 \frac{\partial}{\partial t} \ln t , \quad (58)$$

where

$$\Omega(Q) = aQ + bQ^2 + cQ^3 , \quad (59)$$

$\omega_0 = -\alpha_0/L_0^3$ ,  $a = \alpha_1/L_0^2$ ,  $b = \alpha_2/(2L_0^2)$ , and  $c = \alpha_3/(3L_0^2)$ .

The equation of motion for the auxiliary field, Eq.(56), has the general solution

$$m_q(t) = e^{-\int_{t_0}^t d\tau \omega_q(\tau)} m_q(t_0) . \quad (60)$$

Inserting Eq.(58) into the integral in the exponential gives

$$m_q(t) = e^{-(\Omega(Q(t)) - \Omega(Q(t_0)))} e^{\omega_0 \ln(t/t_0)} m_q(t_0)$$

$$= \left(\frac{t}{t_0}\right)^{\omega_0} e^{-(\Omega(Q(t)) - \Omega(Q(t_0)))} m_q(t_0) . \quad (61)$$

If we then form the auxiliary field correlation function, as defined by the Fourier transform of Eq.(54), we obtain

$$\begin{aligned}
C_0(q, t_1, t_2) &= \left(\frac{t_1 t_2}{t_0^2}\right)^{\omega_0} e^{-(\Omega(Q(t_1)) + \Omega(Q(t_2)) - 2\Omega(Q(t_0)))} \\
&\times C_0(q, t_0, t_0) . \quad (62)
\end{aligned}$$

If we go to the equal-time limit this becomes

$$C_0(q, t, t) = \left(\frac{t}{t_0}\right)^{2\omega_0} e^{-(2\Omega(Q(t)) - 2\Omega(Q(t_0)))} C_0(q, t_0, t_0) . \quad (63)$$

The important autocorrelation function, defined by Eq.(55), is given then by

$$\begin{aligned} S_0(t) &= \int \frac{d^d q}{(2\pi)^d} C_0(q, t, t) \\ &= \frac{1}{L^d(t)} \int \frac{d^d Q}{(2\pi)^d} \left(\frac{t}{t_0}\right)^{2\omega_0} e^{-(2\Omega(Q) - 2\Omega(QL(t_0)/L(t)))} \\ &\quad \times C_0(Q/L(t), t_0, t_0) . \end{aligned} \quad (64)$$

For large  $L(t)$  we can replace

$$C_0(Q/L(t), t_0, t_0) \rightarrow g_0 , \quad (65)$$

where  $g_0$  is characteristic of the initial correlation function, and

$$2\Omega(Q) - 2\Omega(QL(t_0)/L(t)) \rightarrow 2\Omega(Q) , \quad (66)$$

to obtain in Eq.(64)

$$\begin{aligned} S_0(t) &= \frac{g_0}{L^d(t)} \left(\frac{t}{t_0}\right)^{2\omega_0} \int \frac{d^d Q}{(2\pi)^d} e^{-(2\Omega(Q))} \\ &= \frac{g_0}{L^d(t)} \left(\frac{t}{t_0}\right)^{2\omega_0} J_d . \end{aligned} \quad (67)$$

Here we have introduced the constant

$$J_d = \int \frac{d^d Q}{(2\pi)^d} e^{-2\Omega(Q)} . \quad (68)$$

By assumption the auxiliary field scales with the growth law,  $m \approx L$  and  $S_0(t) \approx L^2(t)$ . Using this result back in Eq.(67) gives

$$S_0(t) \approx L^{2\omega_0 - d} \approx L^2 . \quad (69)$$

This fixes the constant  $\omega_0$  to have the value:

$$\omega_0 = \frac{2+d}{6} . \quad (70)$$

Using this result in the scaling regime, the auxiliary field correlation function, given by Eq.(62) can be written in the form

$$C_0(q, t_1, t_2) = \left(\frac{t_1 t_2}{t_0^2}\right)^{\omega_0} e^{-(\Omega(Q(t_1)) + \Omega(Q(t_2)))} g_0 . \quad (71)$$

Eventually we need the inverse Fourier transform of the normalized correlation function

$$f_0(q, t_1, t_2) = \frac{C_0(q, t_1, t_2)}{\sqrt{S_0(t_1)S_0(t_2)}} . \quad (72)$$

Using previous results this can easily be put into the form

$$f_0(q, t_1, t_2) = (L(t_1)L(t_2))^{d/2} \frac{e^{-(\Omega(Q(t_1)) + \Omega(Q(t_2)))}}{J_d} . \quad (73)$$

With  $\Omega(Q)$  given by Eq.(59), we have in the argument of the exponential:

$$\Omega(Q(t_1)) + \Omega(Q(t_2)) = aq(L(t_1) + L(t_2))$$

$$+ bq^2(L^2(t_1) + L^2(t_2)) + cq^3(L^3(t_1) + L^3(t_2)) . \quad (74)$$

If we introduce  $L_T(t_1, t_2)$ , as in Eq.(37), and  $Q = qL_T$ , we obtain

$$\Omega(Q(t_1)) + \Omega(Q(t_2)) = 2aQ\ell_1(t_1, t_2)$$

$$+ 2bQ^2\ell_2(t_1, t_2) + 2cQ^3\ell_3(t_1, t_2) \quad (75)$$

where

$$\begin{aligned} \ell_n(t_1, t_2) &= \frac{1}{2} \left( \frac{L^n(t_1) + L^n(t_2)}{L_T^n(t_1, t_2)} \right) \\ &= \frac{1}{2} \frac{t_1^{n/3} + t_2^{n/3}}{\left(\frac{1}{2}(t_1^{2/3} + t_2^{2/3})\right)^{n/2}} . \end{aligned} \quad (76)$$

For equal times  $\ell_n(t, t) = 1$ , while for  $t_1 \gg t_2$

$$\ell_n(t_1, t_2) = 2^{n/2-1} \quad (77)$$

and  $\ell_2(t_1, t_2) = 1$ . We can then choose  $L_0$  such that  $c = 1/4$ ,  $2b = \mu$  and  $2a = -A$ . We then have the final result

$$f_0(q, t_1, t_2) = (L(t_1)L(t_2))^{d/2} \frac{e^{-N(Q, t_1, t_2)}}{J_d} \quad (78)$$

where

$$N(Q, t_1, t_2) = \frac{1}{2}Q^3\ell_3(t_1, t_2) + \mu Q^2 - A Q \ell_1(t_1, t_2) . \quad (79)$$

The inverse Fourier transform of  $f_0(q, t_1, t_2)$  is the quantity which is related to the  $\sigma$ - correlation function by Eq.(52):

$$f_0(r, t_1, t_2) = \int \frac{d^d q}{(2\pi)^d} e^{-i\vec{q}\cdot\vec{r}} f_0(q, t_1, t_2)$$

$$\begin{aligned}
&= \int \frac{d^d q}{(2\pi)^d} e^{-i\vec{q}\cdot\vec{r}} (L(t_1)L(t_2))^{d/2} \frac{e^{-N(Q,t_1,t_2)}}{J_d} \\
&= \left( \frac{L(t_1)L(t_2)}{L_T^2(t,t_2)} \right)^{d/2} \int \frac{d^d Q}{(2\pi)^d} e^{-i\vec{Q}\cdot\vec{x}} \frac{e^{-N(Q,t,t_2)}}{J_d} \quad (80)
\end{aligned}$$

where  $x = r/L_T$  and now

$$\begin{aligned}
J_d &= \int \frac{d^d Q}{(2\pi)^d} e^{-N(Q,t,t)} \\
&= \int \frac{d^d Q}{(2\pi)^d} e^{-\frac{1}{2}Q^3 - \mu Q^2 + AQ} \quad . \quad (81)
\end{aligned}$$

The Fourier transform of the  $\sigma$ -correlation function is given by:

$$\begin{aligned}
C_\sigma(q, t_1, t_2) &= \int d^d r e^{+i\vec{q}\cdot\vec{r}} \frac{2}{\pi} \sin^{-1} (f_0(r, t_1, t_2)) \\
&= L_T^d \int d^d x e^{+i\vec{Q}\cdot\vec{x}} \frac{2}{\pi} \sin^{-1} (f_0(x, t_1, t_2)) \quad (82)
\end{aligned}$$

and the scaling function appearing in our physical scaling function, Eq.(52), is given by

$$F_\sigma(Q, t_1, t_2) = \int d^d x e^{+i\vec{Q}\cdot\vec{x}} \frac{2}{\pi} \sin^{-1} (f_0(x, t_1, t_2)) \quad (83)$$

where

$$\begin{aligned}
f_0(x, t_1, t_2) &= \left( \frac{L(t_1)L(t_2)}{L_T^2(t_1, t_2)} \right)^{d/2} \\
&\times \int \frac{d^d Q}{(2\pi)^d} e^{-i\vec{Q}\cdot\vec{x}} \frac{e^{-N(Q,t_1,t_2)}}{J_d} \quad . \quad (84)
\end{aligned}$$

## VI. LARGE $Q$ AND SHORT-DISTANCES

One of the main successes of the OJK theory is inclusion of the short distance nonanalytic behavior associated with Porod's law and the Tomita sum rule. We look here at how all of this fits into the present development.

Let us consider Eq.(50) for equal times  $t_1 = t_2 = t \gg t_0$  where

$$F(Q) = F(Q, t, t) = \int_0^1 \frac{dy_1}{y_1} e^{-\int_{y_1}^1 \frac{dy_2}{y_2} H(Q\sqrt{y_2})}$$

$$\begin{aligned}
&\times \int_0^1 \frac{dy_2}{y_2} e^{-\int_{y_2}^1 \frac{dy_3}{y_3} H(Q\sqrt{y_3})} \times H_0(Q\sqrt{y_1}) H_0(Q\sqrt{y_2}) \\
&\times \tilde{\ell}^d(y_1, y_2) F_\sigma(Q\tilde{\ell}(y_1, y_2), ty_1^{3/2}, ty_2^{3/2}) \quad . \quad (85)
\end{aligned}$$

At first sight, since  $H(Q\sqrt{y_1})$  goes at least as fast as  $Q^2$  for large  $Q$ , this integral looks like it gives exponential behavior in  $Q$  for large  $Q$ . Closer inspection shows the asymptotic dependence on  $Q$  is much slower in those regions of the  $y_1$  and  $y_2$  integrals near 1. By expanding  $\tilde{\ell}^d(y_1, y_2) F_\sigma(Q\tilde{\ell}(y_1, y_2), ty_1^{3/2}, ty_2^{3/2})$  about  $y_1 = 1$  and  $y_2 = 1$ , it is not difficult to show, assuming that  $H_0$  and  $H$  increase algebraically with  $Q$  for large  $Q$ , that

$$F(Q) = F_\sigma(Q) \frac{H_0(Q)}{H(Q)} (1 + \mathcal{O}(H(Q))^{-1}) \quad . \quad (86)$$

We will now show that  $F_\sigma(Q)$  falls off algebraically with large wavenumber. This means that the short-distance behavior is controlled, as in the OJK theory, by the auxiliary field  $m$ . We see that the cross-over functions  $H$  and  $H_0$  do not influence this short-distance behavior if we choose  $H = H_0$ . Notice also that it is advantageous to choose  $H(Q)$  to have a high-power of  $Q$  component so one can ignore the corrections to  $F(Q) = F_\sigma(Q)$ . For this reason we keep the  $\gamma_{10}$  term in Eq.(30) and the crossover function  $H(Q)$  does not influence the large  $Q$  behavior of  $F(Q)$  until terms of  $\mathcal{O}(Q^{-14})$ . We do not expect significant variations in our numerical results to depend on whether we keep, for example,  $\gamma_{10}$  or  $\gamma_8$ .

Let us look in more detail at the large  $Q$  behavior of  $F_\sigma(Q)$ . This requires several steps. First we have, using Eq.(52), that in coordinate space

$$F_\sigma(x) = \frac{2}{\pi} \sin^{-1} f_0(x) \quad (87)$$

where  $f_0(x)$  is given by Eq.(84) with  $t_1 = t_2 = t$ :

$$f_0(x) = \int \frac{d^d Q}{(2\pi)^d} e^{-i\vec{Q}\cdot\vec{x}} \frac{e^{-N(Q)}}{J_d} \quad . \quad (88)$$

The short-scaled distance expansion for  $f_0(x)$  can be written in the form

$$f_0(x) = 1 - a_0 x^2 (1 + b_0 x^2 + c_0 x^4 + d_0 x^6 + \dots) \quad . \quad (89)$$

If we define the integrals

$$I_n = \int_0^\infty dQ Q^n e^{-N(Q)} \quad (90)$$

then

$$a_0 = \frac{1}{6} \frac{I_4}{I_2} \quad (91)$$

$$b_0 = -\frac{1}{20} \frac{I_6}{I_4} \quad (92)$$

$$c_0 = \frac{6}{7!} \frac{I_8}{I_4} \quad (93)$$

$$d_0 = -\frac{6}{9!} \frac{I_{10}}{I_4} \quad (94)$$

Inserting Eq.(89) into Eq.(87) and expanding, it is only a matter of stamina to show:

$$F_\sigma(x) = 1 - \alpha x (1 + \beta x^2 + \gamma x^4 + \nu x^6 + \dots) \quad (95)$$

where

$$\alpha = \frac{2}{\pi} \sqrt{2a_0} \quad (96)$$

$$\beta = \frac{a_0}{12} + \frac{b_0}{2} \quad (97)$$

$$\gamma = \frac{c_0}{2} - \frac{b_0^2}{8} + \frac{a_0 b_0}{8} + \frac{3}{160} a_0^2 \quad (98)$$

$$\nu = \frac{d_0}{2} + \frac{a_0^3}{7!} - \frac{4}{105} \beta a_0^2$$

$$+ \frac{25}{56} \beta^2 a_0 + \frac{9}{28} \gamma a_0 - \gamma \beta \quad (99)$$

Thus all of the expansion coefficients for  $F_\sigma(x)$  are known in terms of the parameters  $A$  and  $\mu$  in  $N(Q)$ .

The large- $Q$  behavior of  $F_\sigma(Q)$  follows in three dimensions from the Fourier representation

$$F_\sigma(Q) = \frac{4\pi}{Q} \int_0^\infty dx x \sin(Qx) F_\sigma(x) \quad (100)$$

and, after repeated integrations by parts, one obtains for large  $Q$

$$F_\sigma(Q) = \sum_{n=2}^{\infty} \frac{F_{2n}}{Q^{2n}} \quad (101)$$

where the Porod coefficients are defined by:

$$F_{2n} = 4\pi (-1)^{n+1} \left( \frac{d^{2n-2}}{dx^{2n-2}} (xF_\sigma(x)) \right)_{x=0} \quad (102)$$

Using Eq.(95) in Eq.(102) we easily find

$$F_4 = 8\pi\alpha \quad (103)$$

$$F_6 = -96\pi\alpha\beta \quad (104)$$

$$F_8 = 4\pi 6! \alpha\gamma \quad (105)$$

$$F_{10} = -4\pi 8! \alpha\nu \quad (106)$$

Following Tomita we can show that the lack of even terms in the expansion of  $F(x)$  and  $F_\sigma(x)$  leads to the set of sum rules

$$S_n = \int \frac{d^3 Q}{(2\pi)^3} Q^{2n} \left[ F(Q) - \sum_{m=2}^{n+1} \frac{F_{2m}}{Q^{2m}} \right] = 0 \quad (107)$$

If we set  $F(Q) = F_\sigma(Q)$  in Eq.(107), because of Eq.(95), the sum rules are obeyed identically. However, if we insert  $F(Q)$  given by Eq.(85) into Eq.(107), there is no reason in general to expect the sum rules to be satisfied. Indeed this gives a set of conditions on  $F(Q)$  which can be used, along with the normalization

$$S_0 = \int \frac{d^3 Q}{(2\pi)^3} F(Q) - 1 = 0 \quad , \quad (108)$$

to determine the parameters  $A$ ,  $\mu$  and those determining  $H(Q)$ .

## VII. DETERMINATION OF THE SCALING FUNCTION

The equal-time scaling function  $F(Q)$  given by Eq.(50) is a function of the  $\gamma_n$ ,  $\gamma_n^0$ ,  $A$  and  $\mu$ . Our basic assumption is that our model is characterized by the normalization Eq.(108) and the set of sum rules given by Eq.(107). Thus we have an infinite set of parameters and an infinite set of conditions. Here we work out the truncated theory where we use the four conditions  $S_i = 0$ , for  $i = 0, 1, 2, 3$  to determine the parameters  $P = \{\gamma_2, \gamma_{10}, A, \mu\}$  with  $\gamma_n = \gamma_n^0$ . Thus there are no free parameters.

One then has a rather complicated numerical minimization problem. First assume values of the

four parameters  $P^{(1)}$  and compute  $F^{(1)}(Q)$  and simultaneously the four sum rules  $S_n^{(1)}$ . Then choose another set  $P^{(2)}$  and determines the set  $S_n^{(2)}$ . One then needs a measure, like

$$\mathcal{J}^{(i)} = \sum_{n=0}^3 \left( S_n^{(i)} \right)^2 , \quad (109)$$

to minimize. Thus, if  $\mathcal{J}^{(2)} < \mathcal{J}^{(1)}$ , the set of parameters  $P^{(2)}$  is preferred over the set  $P^{(1)}$ . One then iterates this process until it converges to a selected *fixed-point* set of values of the parameters  $P^*$  and scaling function  $F^*(Q)$ .

In the numerical determination of the  $S_n$  it is important to take into account that these integrals are slowly converging for large wavenumbers. Suppose we have integrated a sum rule out to a cutoff wavenumber  $Q_M$  and obtain a contribution  $S_n^{Q_M}$ . If  $Q_M$  is large enough, the system is dominated by the large- $Q$  power-law behavior as in Porod's law and one can evaluate the remaining contribution to the integral in terms of an appropriate Porod coefficient:

$$S_n = S_n^{Q_M} + \frac{F_{2n+2}}{2\pi Q_M} . \quad (110)$$

The determination of the  $S_n^{Q_M}$  is a challenging numerical problem since one must perform multiple nested integrations  $y_1, y_2$  and internal Fourier transforms and still maintain sufficient numerical accuracy that the Porod coefficients  $F_{2n}$  can be extracted and the sum rules constructed. Thus the choice  $Q_M$  must be monitored carefully when determining  $S_n^{Q_M}$ .

As a result of extensive iterations we arrive at the fixed point values [32] for the parameters:  $\gamma_2 = 1.4994 \dots$ ,  $\gamma_{10} = 0.1232 \dots$ ,  $A = 6.395 \dots$ , and  $\mu = 0.2162 \dots$ . In Fig. 1 we plot the determined scaling function  $F(Q)$  versus the accurate numerical results of Oono and Shinozaki [22]. Notice that the structure factor is normalized by the position and height of the first maximum. The agreement for small  $Q$  is very good and the width of the peak is in good agreement with the numerical results. In Fig.2 we plot  $Q^4 F(Q)$  for the theory and the same set of numerical results. Again overall agreement is good. The value of the Porod coefficient  $F_4$  for the theory and simulation are in excellent agreement. The feature of a second maximum is present in the theory but its position and width are not in very good agreement with the numerical results. In Figs.3-6

we plot the running contributions to the sum rules to give a feeling for the degree of convergence of the numerical procedure described above. To obtain the complete contribution to the sum rules we must add the last term in Eq.(110). The analytically determined Porod coefficients needed in completing the analysis are given by  $F_4 = 21.87$ ,  $F_6 = 19.72$ ,  $F_8 = -52.85$  and  $F_{10} = -25.41$ .

The results here should be compared with previous direct calculations of the  $F(Q)$ . In Ref.([11]) the calculated  $F(Q)$  obeyed Porod's law, did not obey the lowest Tomita sum rule, went as  $Q^2$  for small  $Q$  and gave a width significantly too broad compared to numerical results. In Ref.([12]) the large and small  $Q$  limits were in agreement with expectations but the Tomita sum rule was not satisfied and the width of the scaling function was significantly *too narrow*. In Ref.([31]) the authors obtained a scaling function which satisfied Porod's law, the Tomita sum rules and was fit to the numerically determined width. Unfortunately, this work not only did not give the  $Q^4$  small  $Q$  behavior for  $F(Q)$ , it did not satisfy the conservation law,  $F(0) > 0$ .

## VIII. AUTOCORRELATION FUNCTION EXPONENTS

We turn next to a discussion of the two-time order parameter correlation function. In this case we focus on the behavior of the autocorrelation function, which, when both  $t_1$  and  $t_2$  are in the scaling regime, is given by

$$\begin{aligned} \Psi(t_1, t_2) &= \langle \psi(\mathbf{r}, t_1) \psi(\mathbf{r}, t_2) \rangle \\ &= \int \frac{d^d q}{(2\pi)^d} C(q, t_1, t_2) = \psi_0^2 \int \frac{d^d Q}{(2\pi)^d} F(Q, t_1, t_2) \\ &= \psi_0^2 \int \frac{d^d Q}{(2\pi)^d} \int_{(t_0/T)^{2/3}}^{(t_1/T)^{2/3}} \frac{dy_1}{y_1} U_q(t_1, T y_1^{3/2}) \\ &\quad \times \int_{(t_0/T)^{2/3}}^{(t_2/T)^{2/3}} \frac{dy_2}{y_2} U_q(t_2, T y_2^{3/2}) H_0(Q\sqrt{y_1}) H_0(Q\sqrt{y_2}) \\ &\quad \times \ell^d(y_1, y_2) F_\sigma(Q\ell(y_1, y_2), T y_1^{3/2}, T y_2^{3/2}) . \quad (111) \end{aligned}$$

In the regime  $t_1 \gg t_2$ ,  $\Psi(t_1, t_2)$  is expected to take the form [1]

$$\Psi(t_1, t_2) \approx \left( \frac{L(t_2)}{L(t_1)} \right)^\lambda \quad (112)$$

and the exponent  $\lambda$  is distinct from the growth law. It is not difficult to extract  $\lambda$  from Eq.(111).

For  $t_1 \gg t_2$  the integral over  $y_2$  is restricted to small values and the autocorrelation function can be put into the form

$$\begin{aligned} \Psi(t_1, t_2) &= \psi_0^2 \int \frac{d^d Q}{(2\pi)^d} \int_0^2 \frac{dy_1}{y_1} e^{\left( - \int_{y_1}^2 \frac{dy_2}{y_2} H(Q\sqrt{y_1}) \right)} \\ &\times H_0(Q\sqrt{y_1}) \int_0^{2(t_2/t_1)^{2/3}} \frac{dy_2}{y_2} \gamma_2 Q^2 y_2 \\ &\times \tilde{\ell}^d(y_1, 0) F_\sigma(Q\tilde{\ell}(y_1, 0), T y_1^{3/2}, T y_2^{3/2}) \quad . \quad (113) \end{aligned}$$

The key observation is that for  $t_1 \gg t_2$  the auxiliary field correlation function is small and we can linearize Eq.(83) relating the order parameter and the auxiliary field correlation function to obtain

$$F_\sigma(Q, t_1, t_2) \approx \frac{2}{\pi} f_0(Q, t_1, t_2) \quad , \quad (114)$$

where

$$f_0(Q, t_1, t_2) = \left( \frac{L(t_1)L(t_2)}{L_T^2} \right)^{d/2} \frac{e^{-N(Q, t_1, t_2)}}{I_d} \quad . \quad (115)$$

Then to leading order for  $t_1 \gg t_2$

$$\begin{aligned} f_0(Q, t_1, t_2) &= \left( \frac{2L(t_2)}{L(t_1)} \right)^{d/2} \frac{e^{-\frac{1}{\sqrt{2}}(Q^3 + \sqrt{2}\mu Q - A Q)}}{I_d} \quad . \quad (116) \end{aligned}$$

Inserting this result back into Eq.(113), we find that the overall time dependence is governed by the  $y_2$  integral given by

$$\int_0^{2(L(t_2)/L(t_1))^2} dy_2 y_2^{d/4} \approx (L(t_2)/L(t_1))^{d/2+2} \quad (117)$$

and we can identify [33]  $\lambda = d/2 + 2$ . This result corresponds to the lower bound established by Yeung, Rao and Desai [18].

If  $t_2 = t_0$  then the analysis must be altered. The key point is that one must keep the first term in Eq.(24) and the dominant term for long times is the correlation between the second term in Eq.(24)

for the field at  $t_1$  and the initial correlation. Then one has

$$C(q, t_1, t_0) = \int_{t_0}^{t_1} d\bar{t} U_q(t_1, \bar{t}) N_q(\bar{t}) < \sigma_q(\bar{t}) \sigma_{-q}(\bar{t}_0) > \quad (118)$$

The analysis of this quantity for large  $t_1$  follows the earlier analysis with respect to rescaling of the  $t_1$  dependence. The main difference in the calculation is that there is no  $y_2$  integration as in the  $t_2 \gg t_0$  case and one has the direct factor as in Eq.(116) which leads to the behavior

$$\Psi(t_1, t_2) \approx (L_1)^{-d/2} \quad . \quad (119)$$

In this case we again obtain that the exponent is given by the lower bound value  $\lambda_0 = d/2$  found by Yeung, et al [18].

## IX. DISCUSSION

In this paper we have developed a theory of the phase-ordering kinetics of the CH model which plays a role similar to the OJK theory for the NCOP case. The theory includes all of the desired features discussed in section 2 including the elusive Tomita sum rule. It is also in good numerical agreement with the best available numerical results. The theory, because of the nonlocal mapping onto the auxiliary field, is much more difficult to treat analytically when compared to the OJK theory. Nevertheless it seems to work well. While we are able to extract the apparently mean field values for the nonequilibrium exponents  $\lambda$  and  $\lambda_0$ , it looks very difficult to include the nonlinear terms in the  $m$  field necessary to give the higher-order corrections for the exponents.

There are several directions in which this work can be extended. One can, in principle, include additional  $\gamma_n$  parameters in the model and satisfy higher order sum rules. This will be numerically difficult and probably will not improve the scaling function significantly. While the detailed analysis here has been for three dimensions, with only a modest amount of additional analytical work, the selection process can be applied to two dimensional systems. The most interesting new direction is to apply this same theory to off critical quenches. The expectation is that the scaled structure factor broadens significantly as one moves away from critical quenches. It will be interesting to see how well the theory describes the system as one moves toward the

coexistence curve and the regime where the Lifshitz-Slyosov-Wagner theory [34] is applicable.

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[1] A. J. Bray, *Adv. Phys.* **43**, 357 (1994).

[2] T. Ohta, D. Jasnow, and K. Kawasaki, *Phys. Rev. Lett.* **49**, 1223 (1983).

[3] G. Porod, *Kolloid Z.* **124**, 83 (1951); **125**, 51 (1952).

[4] P. Debye, H. R. Anderson and H. Brumberger, *J. Appl. Phys.* **28**, 679 (1957).

[5] G. Porod, in **Small Angle X-Ray Scattering**, ed. by O. Glatter and L. Kratky (Academic, N.Y., 1982).

[6] Y. Oono and S. Puri, *Phys. Lett. B* **7**, 861 (1988).

[7] C. Yeung and D. Jasnow, *Phys. Rev. B* **42**, 10523 (1990)

[8] S. Puri and C. Roland, *Phys. Rev. A* **51**, 500 (1990).

[9] A. J. Bray and K. Humayun, *Phys. Rev. E* **48**, R1609 (1993).

[10] G. F. Mazenko, *Phys. Rev. B* **42**, 4487 (1990).

[11] G. F. Mazenko, *Phys. Rev. B* **43**, 5747 (1991).

[12] G. F. Mazenko, *Phys. Rev. E* **50**, 3485 (1994).

[13] C. Yeung, Y. Oono, and A. Shinozaki, *Phys. Rev. E* **49**, 2693 (1994).

[14] G. F. Mazenko, *Phys. Rev. E* **58**, 1543 (1998).

[15] G. F. Mazenko, *Phys. Rev. E* **61**, 1088 (1998).

[16] J. W. Cahn and J.E. Hilliard, *J. Chem. Phys.* **28**, 258 (1958).

[17] H. Tomita, *Prog. Theor. Phys.* **72**, 656 (1984); **75**, 482 (1986).

[18] C. Yeung, M. Rao and R.C. Desai, *Phys. Rev. E* **53**, 3073 (1996).

[19] J. Marro, J.L. Lebowitz, and M.H. Kalos, *Phys. Rev. Lett.* **43**, 282 (1979).

[20] K. Binder and D. Stauffer, *Phys. Rev. Lett.* **33**, 1006 (1974).

[21] H. Furukawa, *Prog. Theor. Phys.* **59**, 1072 (1978).

[22] A. Shinozaki and Y. Oono, *Phys. Rev. Lett.* **66**, 173 (1991).

[23] I.M. Lifshitz and V.V. Slyozov, *J. Phys. Chem. Solids* **19**, 35 (1961); C. Wagner, *Z. Elektrochem.* **65**, 581 (1961).

[24] J. S. Langer and L. A. Turski, *Acta. Metall.* **25**, 1113 (1977).

[25] A. Rutenberg and A.J. Bray, *Phys. Rev. E* **51**, 5499 (1995).

[26] A. J. Bray, *Phys. Rev. E* **58**, 1508 (1998).

[27] C. Yeung, *Phys. Rev. Lett.* **61**, 1135 (1988).

[28] A. J. Bray and S. Puri, *Phys. Rev. Lett.* **67**, 2670 (1991).

[29] There are not very many possibilities for quantities which are or  $\mathcal{O}(1)$  if they are to be built out of  $\sigma$  and  $\psi$ . If one allows gradients then one has quantities like  $(\nabla m)^2$  as discussed in Ref. ([14]).

[30] This new mapping, unlike the case discussed in Ref. ([13]), is nonlocal in both space and time.

[31] T. Ohta and H. Nozaki, in **Space-Time Organization in Macromolecular Fluids**, Edited by F. Tanaka, M. Doi, and T. Ohta, Springer Series in Chemical Physics Vol 51, ( Springer-Verlag, Berlin, 1989).

[32] In order to speed up the convergence we have allowed the ratio  $r = H_0(Q)/H(Q)$  to float. It takes on the fixed point value 1.0055... in agreement with the assumption that it can be chosen to be 1.

[33] The integration over  $y_1$  is well behaved at its lower limit if  $d < 4$ .

[34] T. Ohta, *Prog. Thero. Phys.* **71**, 1409 (1984).

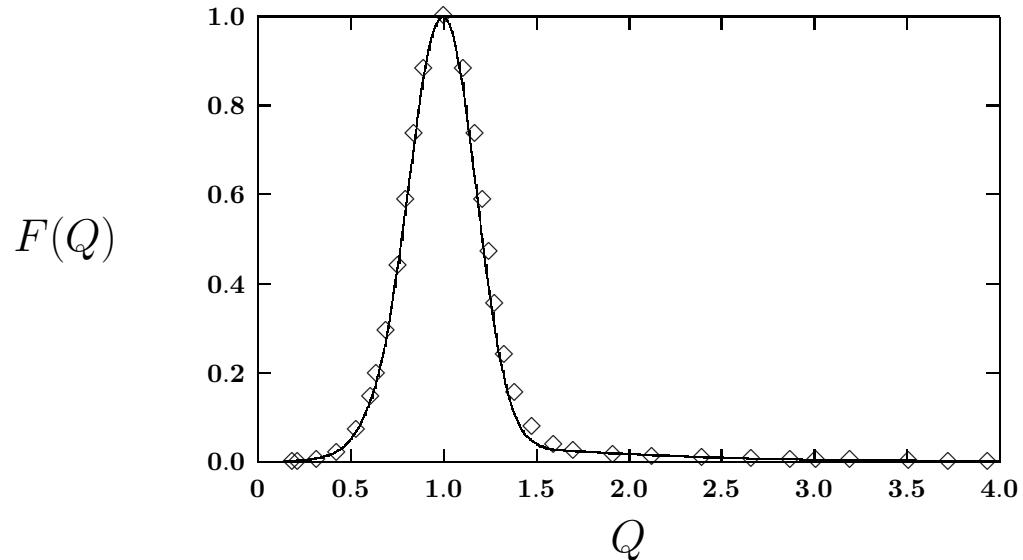


FIG. 1. Plot of scaled structure factor versus scaled wavenumber. Solid line represent the theory and the squares the numerical results from Ref.([22])

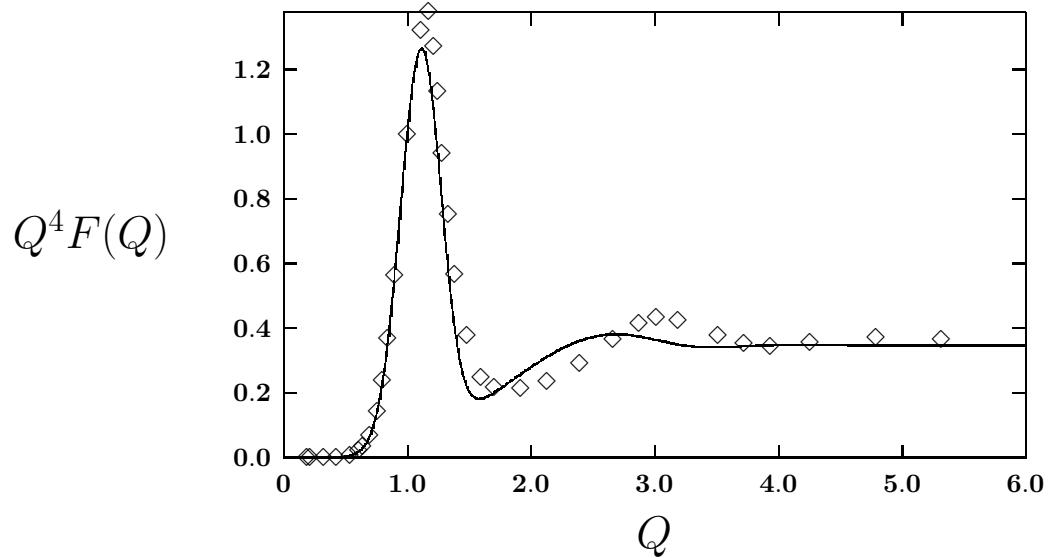


FIG. 2. Porod plot of scaled structure factor versus scaled wavenumber. Solid line represent the theory and the squares the numerical results from Ref.([22])

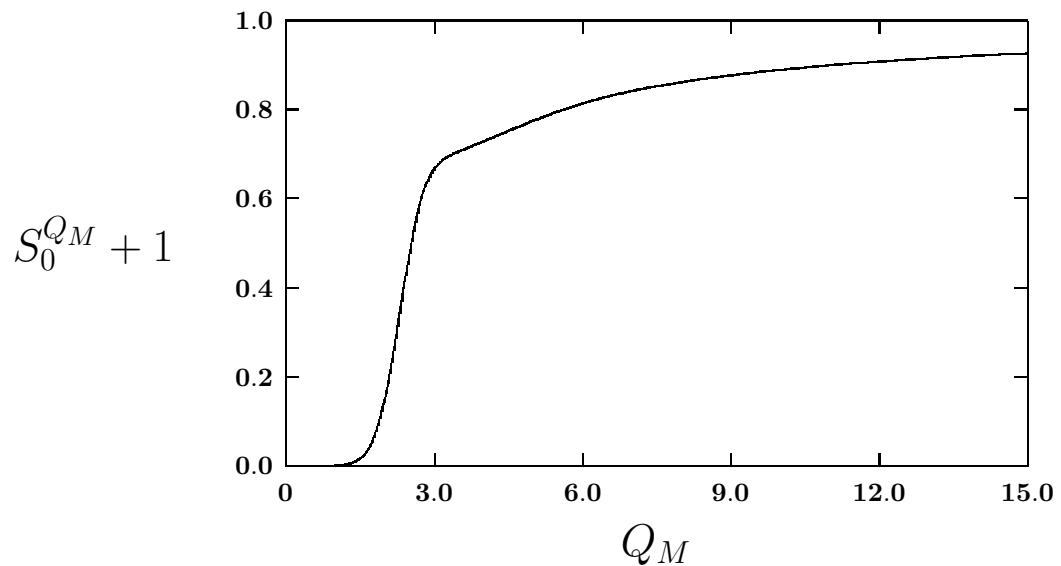


FIG. 3. Plot of normalization of structure factor versus cutoff wavenumber

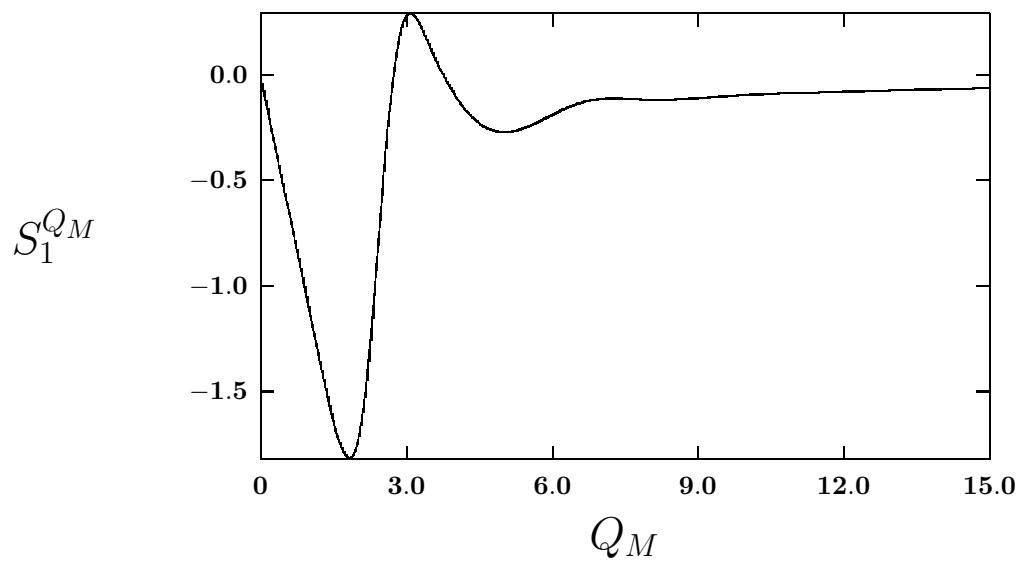


FIG. 4. Plot of sum rule  $S_1^{Q_M}$  versus cutoff wavenumber

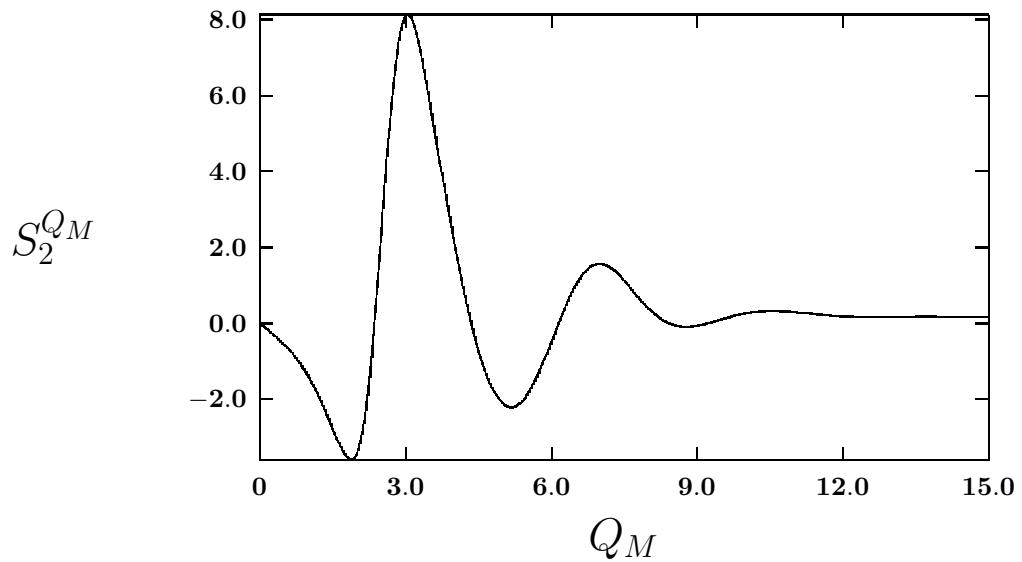


FIG. 5. Plot of sum rule  $S_2^{QM}$  versus cutoff wavenumber

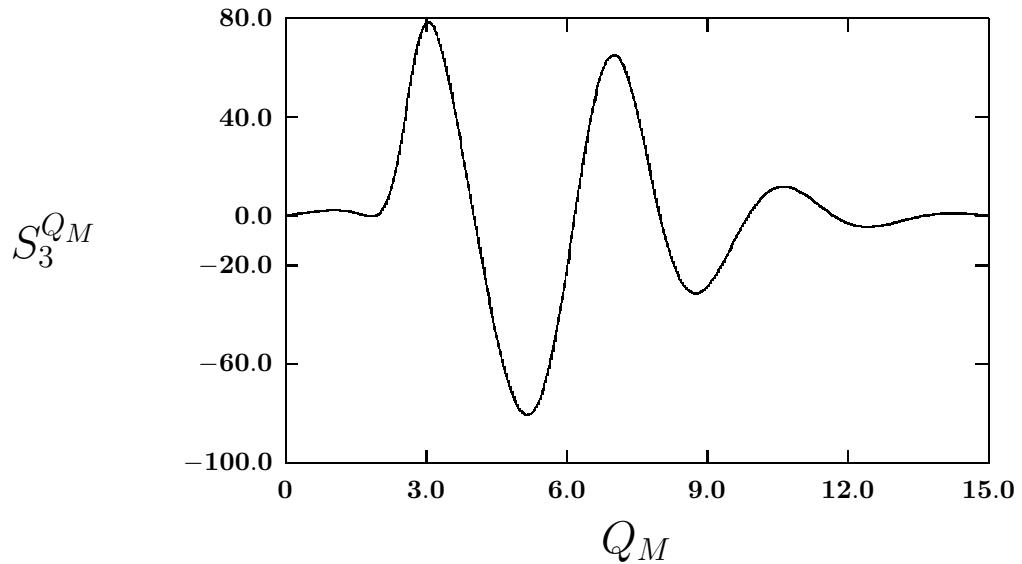


FIG. 6. Plot of sum rule  $S_3^{QM}$  versus cutoff wavenumber